Exercise 1
Computational Methods for the Interaction of Light and Matter (WS2019/20)

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Numerical integration of the Formal Transfer Equation

As discussed in the lecture, the *formal transfer equation (FTE)* along a single ray with coordinate s is

$$\frac{dI(s)}{ds} = \alpha(s)\big(S(s) - I(s)\big) \tag{1}$$

In this exercise we will not concern ourselves (yet) with scattering. So the source function equals the Planck function, $S(s) = B(s)$. For simplicity we will, at first, use non-physical units. Let us give the function $B(s)$ a Gaussian shape as follows

$$B(s) = B_0 + (B_1 - B_0) \exp\left(-\frac{1}{2}\frac{s^2}{w^2}\right) \tag{2}$$

were B_0, B_1 and w are parameters of our model. For the extinction coefficient $\alpha(s)$ let us take a simple box-function (i.e. a cloud with homogeneous density):

$$\alpha(s) = \begin{cases} A & \text{for } |s| \le L \\ 0 & \text{for } |s| > L \end{cases} \tag{3}$$

As a starting value of the intensity (at $s < -L$) we have $I = I_{\text{in}}$. We now want to compute the outcoming intensity I_{out} (i.e. the intensity at $s > L$).

As default parameters let us choose $B_0 = 1$, $B_1 = 3$, $I_{\text{in}} = 0$, $w = 1$, $L = 3$ and $A = 1$, but we will vary some of these parameters in the exercise below.

Let us solve the FTE *numerically.* We set up a *grid* in s within the domain $s \in [-L, L]$ with $N = 100$ grid points evenly spaced.

1. For the default case, what is the total optical depth along the ray?
2. Program a function that integrates the FTE numerically for the above problem, and returns the values of $I(s)$ at all grid points. Use the simple *forward Euler* algorithm for that. Apply it to the default problem, and plot the result as a function of s.
3. Now set $A = 10$, and try again. Explain the differences to the $A = 1$ case.
4. Now set $A = 100$, and try again. You will see that the forward Euler algorithm will become numerically unstable. Explain what happens, and why.

Now let's find a solution to the numerical instability seen above, because we want to have an algorithm that works for *any* physically realistic case. The idea we will explore is to use *piecewise analytic* solutions. Let us assume that between neighboring grid points i and $i + 1$ the value of $B(s)$ is constant. Let us call this value $B_{i+1/2}$, for notational simplicity. We can either set $B_{i+1/2} = B(s_{i+1/2})$, with $s_{i+1/2} = (s_i + s_{i+1})/2$, or we simply average by setting $B_{i+1/2} = (B_i + B_{i+1})/2$. Either way is equally good or bad.

5. Using the analytic solution of the FTE along each segment connecting consecutive gridpoints, design an algorithm for integration of the FTE that is *unconditionally stable.*

6. Implement this into your program, in such a way that the user of your integration function can choose which method of integration to use.

7. Test that the method indeed works also for the $A = 100$ case, and that it produces the result you would expect.

This first order integration method is very robust: If you use this algorithm only for computing the emerging (observable) intensity $I_{\rm out}$, then this method, while not particularly accurate, at least gives reasonable results. However, as we will encounter later in the course: when using the FTE for solving scattering problems in the high-optical-depth regime, simple first order integration will not properly account for radiative diffusion, and can thus produce wrong (not just inaccurate, but entirely wrong) results for the scattering problem.

Can we do better? Yes we can. The next best thing to assuming B to be constant between grid points, is to assume B to be a linear interpolation between B_i and B_{i+1}. We will, however, do this linear interpolation not in the coordinate s, but in the coordinate τ, which is defined by

$$d\tau = \alpha(s)ds \tag{4}$$

In other words: we will use the optical depth *as a coordinate.* The FTE then becomes:

$$\frac{dI(\tau)}{d\tau} = S(\tau) - I(\tau) \tag{5}$$

Now let us derive the expression for the analytic solution of the FTE across a single grid interval $[\tau_i, \tau_{i+1}]$ assuming $S(\tau)$ to be a *linear* function of τ. Let us, for simplicity, assume that

$$\tau_i = 0, \qquad \tau_{i+1} = \Delta\tau \tag{6}$$

where $\Delta\tau$ is the grid spacing. Since we can always choose the $\tau = 0$ point where we like, this assumption is without loss of generality, and it will save us a lot of unnecessary terms that cancel out at the end. So we can write for this interval:

$$S(\tau) = \left(1 - \frac{\tau}{\Delta\tau}\right) S_i + \left(\frac{\tau}{\Delta\tau}\right) S_{i+1} \tag{7}$$

8. Show that the general solution of the FTE within this interval is then

$$I(\tau) = Ke^{-\tau} + \left(\frac{S_{i+1} - S_i}{\Delta\tau}\right)\tau + \left(S_i - \frac{S_{i+1} - S_i}{\Delta\tau}\right) \tag{8}$$

9. Show that the value of I at the end of the interval (i.e. for τ set to $\Delta\tau$) reads:

$$I_{i+1} = I_i e^{-\Delta\tau} + \left(\frac{1 - (1 + \Delta\tau)e^{-\Delta\tau}}{\Delta\tau}\right) S_i + \left(\frac{\Delta\tau - 1 + e^{-\Delta\tau}}{\Delta\tau}\right) S_{i+1} \tag{9}$$

   This is the second-order integration scheme of Olsen & Kunasz 1987, J. Quant. Spectros. Radiat. Transfer 38, 325 (they also presented a third-order version).

10. Implement this into your code, and see how it performs.